

Hierarchical Theory of Quantum Adiabatic Evolution

Qi Zhang,^{1,2} Jiangbin Gong,^{3,4} and Biao Wu^{5,6,*}

¹College of Science, Zhejiang University of Technology, Hangzhou 310014, China

²International Joint Research Laboratory for Quantum Functional Materials of Henan Province and School of Physics and Engineering Zhengzhou University, Henan 450001, China

³Department of Physics and Centre for Computational Science and Engineering, National University of Singapore, 117542, Singapore

⁴NUS Graduate School for Integrative Sciences and Engineering, Singapore 117597, Singapore

⁵International Center for Quantum Materials, Peking University, Beijing 100871, China

⁶Collaborative Innovation Center of Quantum Matter, Beijing, China

(Dated: February 24, 2014)

Quantum adiabatic evolution is a dynamical evolution of a quantum system under slow external driving. According to the quantum adiabatic theorem, no transitions occur between non-degenerate instantaneous eigen-energy levels in such a dynamical evolution. However, this is true only when the driving rate is infinitesimally small. For a small nonzero driving rate, there are generally small transition probabilities between the energy levels. We develop a theory to address the small deviations from the quantum adiabatic theorem order by order. A hierarchy of Hamiltonians are constructed iteratively with the zeroth-order Hamiltonian being the original system Hamiltonian. The k th-order deviations are governed by a k th-order Hamiltonian, which depends on the time derivatives of the adiabatic parameters up to the k th-order. Two simple examples, the Landau-Zener model and a spin-1/2 particle in a rotating magnetic field, are used to illustrate our hierarchical theory.

PACS numbers: 03.65.Vf, 05.40.-a, 05.45.-a, 37.10.Gh, 45.20.Jj

I. INTRODUCTION

Quantum evolution under external adiabatic driving has been of fundamental interests to physicists. Born and Fock proved the quantum adiabatic theorem shortly after the discovery of the Schrödinger equation [1]. This theorem states that no transition occurs between instantaneous eigen-energy levels in a system under adiabatic driving. However, this is only true when the external driving is infinitesimally slow. With a slow but finite external driving, there is generally small tunneling between energy levels. There has been a great deal of effort to address this small deviation from the quantum adiabatic theorem [2–7]. However, a completely successful theory is yet to be developed. This failure has led to a controversy on the validity of the quantum adiabatic theorem [8–11]. With the success of the quantum adiabatic algorithm in quantum computing, this issue has become also important in a practical sense [12, 13]. Our theory should lead to a better assessment and control of the errors in the quantum adiabatic computing.

In this work we present a theory to address the deviation from the quantum adiabatic theorem. We construct iteratively a hierarchy of Hamiltonians with the zeroth-order Hamiltonian being the original Hamiltonian. The deviations of the k th order are the adiabatic invariances of the k th-order Hamiltonian while the adiabaticity of the k th-order Hamiltonian is determined by the time deriva-

tives of the external parameters (denoted R) up to the k th-order. Within this theoretical framework, the deviations from the quantum adiabatic theorem can be computed to arbitrary order iteratively. The theory breaks down at the k th-order when the k th-order time derivative of the external parameters becomes relatively large. We use two simple examples, the Landau-Zener model and the spin-1/2 under a rotating magnetic field, to illustrate our hierarchical theory.

Our hierarchical theory establishes an intuitive picture for quantum adiabatic evolution. At the zeroth-order, the adiabatic evolution is a smooth curve of instantaneous eigenstates in the projective Hilbert space where the overall phase is removed. We call the smooth curve adiabatic trajectory (see Fig.1). At the first order, this adiabatic trajectory is shifted by a small amount that is proportional to the first time derivative of external parameters ($\dot{R} = dR/dt$). At the second order, the adiabatic trajectory is shifted again by a small amount that is proportional to \dot{R}^2 or other possible second-order small parameters, such as \ddot{R} . This intuitive picture is illustrated in Fig. 1. There may or may not be small oscillations around the shifted adiabatic trajectory depending on the detail how R changes with time.

Technically we take advantage of two facts to develop our theory. First, we use the superposition principle, which allows us to focus on the adiabatic evolution of each individual energy eigenstate. Second, we use the classical Hamiltonian formulation of the Schrödinger equation [14, 15]. In this formalism, an energy eigenstate is mapped into an elliptic fixed point in the corresponding projective Hilbert space. Note that this classical formulation is purely mathematical and is *not* the traditional

*Electronic address: wubiao@pku.edu.cn

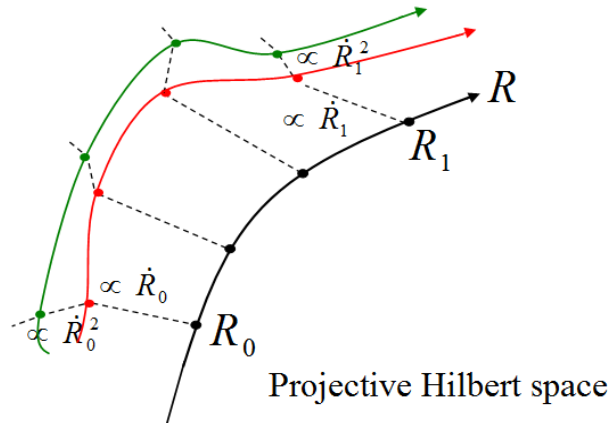


FIG. 1: (Color online) The adiabatic trajectories of different orders in the projective Hilbert space. The black line is for the zeroth-order, the red line for the first-order, and the dark green line for the second-order. The difference between the zeroth-order and the first-order trajectories is proportional to \dot{R} while the difference between the first-order and the second-order trajectories is proportional to \dot{R}^2 . The possible small oscillations around the adiabatic trajectories of the first and second orders are omitted for clarity.

semiclassical limit $\hbar \rightarrow 0$.

II. CLASSICAL HAMILTONIAN FORMULATION OF THE SCHRÖDINGER EQUATION

We consider a quantum system described by the Hamiltonian $\hat{H}_0(R)$, where $R = R(t)$ represents time-dependent parameters in an adiabatic protocol. As normally assumed for quantum adiabatic evolutions [1], $\hat{H}_0(R)$ has a discrete non-degenerate spectrum during the entire control protocol. Further, the rate of change in R is small as compared with the transition frequencies of the system. Deviations from the quantum adiabatic theorem are expected so long as the protocol is not executed in the mathematical limit $\dot{R} \rightarrow 0$. The aim of this work is to develop a general and systematic framework to quantitatively describe such deviations.

Though our consideration can be extended to cases with a Hilbert space of infinite dimensions, for convenience we assume $\hat{H}_0(R)$ lives in a finite n -dimensional Hilbert space. $\hat{H}_0(R)$ can thus be expressed as a R -dependent $n \times n$ Hermitian matrix. We find it mathematically more convenient to use the classical Hamiltonian formulation for the Schrödinger equation [14, 15]. We express the quantum state with an n -component wavefunction $|\psi\rangle = (c_1, c_2, \dots, c_n)^T$ and Define $n - 1$ pairs of canonical variables

$$p_i = \arg(c_{i+1}) - \arg(c_1), \quad q_i = |c_{i+1}|^2, \quad (1)$$

with $i = 1, 2, \dots, n-1$. By construction, the Schrödinger equation then yields the following Hamilton's equations of motion,

$$\frac{dp_i}{dt} = -\frac{\partial H_0(R)}{\partial q_i}, \quad \frac{dq_i}{dt} = \frac{\partial H_0(R)}{\partial p_i}, \quad (2)$$

where the classical Hamiltonian $H_0(R)$ is obtained from the quantum Hamiltonian $\hat{H}_0(R)$ as

$$H_0(R) = \langle \psi | \hat{H}_0(R) | \psi \rangle. \quad (3)$$

As the overall phase is removed, the phase space in this classical formalism is just the projective Hilbert space. This alternative formalism of the Schrödinger equation will allow us to exploit powerful and familiar tools in classical mechanics in our analysis.

the overall phase of the wavefunction, or equivalently $\arg(c_1)$, is removed in Eq. (2) [14, 15]

It is particularly interesting to look at eigenstates. In the original Schrödinger equation picture, an energy eigenstate of $\hat{H}_0(R)$ at a fixed R simply develops a trivial overall phase. Since the overall phase is discarded in our formalism, such an eigenstate evolution is mapped to a fixed point in the classical phase space of $H_0(R)$. The issue of the adiabatic following with the instantaneous energy eigenstates of $\hat{H}_0[R(t)]$ now becomes the issue of the adiabatic following with the instantaneous fixed points of $H_0[R(t)]$.

In principle, the time evolution emanating from an arbitrary initial state as a superposition of different energy eigenstates can be considered. However, the linearity of the original Schrödinger equation indicates that it suffices to study initial states that are energy eigenstates of $\hat{H}_0[R(0)]$ at $t = 0$. As such, in our classical formalism we only need to consider those initial conditions that are fixed points in the phase space.

One final technical comment is in order. The mapping from the wavefunction components c_i to phase space variables (p_i, q_i) [see Eq. (1)] becomes ambiguous when any one of the wavefunction component c_i becomes zero. Fortunately, this ambiguity can be easily overcome by adopting a different representation to re-express the wavefunction. For example, c_1 in Eq. (1) is used to remove the overall wavefunction phase. If $c_1 = 0$, one can always select another nonzero c_i to carry out a similar mapping.

III. FIRST ORDER DEVIATIONS

As the generalization to arbitrary dimensions is straightforward, we consider a quantum system with a two-dimensional Hilbert space for the rest of the paper. With $n = 2$ the Hamilton's equations of motion in Eq. (2) only involve one pair of canonical variables q_1 and p_1 . The phase space is hence also two-dimensional. For clarity we drop the subscript 1 hereafter. A R -dependent fixed point in the phase space is denoted as $[\bar{p}(R), \bar{q}(R)]$.

There are two fixed points corresponding to two energy eigenstates of $\hat{H}_0(R)$.

According to the quantum adiabatic theorem, under a sufficiently slow protocol $R = R(t)$, the dynamics emanating from an energy eigenstate will follow the instantaneous energy eigenstates. With the removal of the overall phase, this dynamics is completely described by the smooth curve of instantaneous energy eigenstates in the projective Hilbert space. We shall call it adiabatic trajectory (see Fig. 1). In the classical formalism, this adiabatic trajectory is the smooth curve of instantaneous fixed points in the phase space. However, in a realistic protocol where $R(t)$ changes slowly with a nonzero rate, there should be a deviation from this picture of perfect adiabatic following.

There were studies on the small deviations from what the adiabatic theorem predicts. It was done in special classical systems and the small deviations were found to pollute the Hannay's angle [16–18]. Recently, the first-order deviation was studied in nonlinear quantum adiabatic evolutions [19], where the result was used successfully to predict a new kind of geometric phase beyond the traditional Berry phase. As their focus was on the global effects of the deviations, detailed dynamics of the deviation was not considered. Our work conducts a systematic study of the quantum adiabatic evolution and reveals its hierarchical structure. Our results can be easily generalized to classical systems and nonlinear quantum systems.

With possible deviations from the instantaneous fixed points $[\bar{q}(R), \bar{p}(R)]$, the actual adiabatic trajectory in the phase space can be written as

$$p(t) = \bar{p}[R(t)] + \delta p, \quad q(t) = \bar{q}[R(t)] + \delta q, \quad (4)$$

with $(\delta p, \delta q)$ being time-dependent deviations from the ideal adiabatic trajectory $[\bar{p}(R), \bar{q}(R)]$. This section is mainly to develop a theory to understand the behavior of $(\delta p, \delta q)$ to the first order of \dot{R} .

As a preparation we first consider the case when R is fixed. Using Hamilton's equations of motion and Taylor expanding $\frac{\partial H_0(R)}{\partial p}$ and $\frac{\partial H_0(R)}{\partial q}$ to the first order of $(\delta p, \delta q)$, we have

$$\begin{pmatrix} \frac{dp}{dt} \\ \frac{dq}{dt} \end{pmatrix} = \Gamma_0 \begin{pmatrix} \delta p \\ \delta q \end{pmatrix}, \quad (5)$$

where

$$\Gamma_0 = \begin{pmatrix} -\frac{\partial^2 H_0}{\partial q \partial p} & -\frac{\partial^2 H_0}{\partial q \partial q} \\ \frac{\partial^2 H_0}{\partial p \partial p} & \frac{\partial^2 H_0}{\partial p \partial q} \end{pmatrix}_{p=\bar{p}, q=\bar{q}} \quad (6)$$

is an R -dependent matrix obtained from the second-order derivatives of $H_0(R)$. The terms with first-order derivatives of $H_0(R)$ do not appear on the right-hand side of Eq. (5) simply because $[\bar{q}(R), \bar{p}(R)]$ is a fixed point. All higher-order terms are neglected here.

We now consider the dynamics of $(\delta q, \delta p)$ in the control protocol where $R = R(t)$ changes slowly with time. In this case, we have

$$\begin{aligned} \frac{dp}{dt} &= \frac{\partial \bar{p}(R)}{\partial R} \dot{R} + \frac{d\delta p}{dt} \\ \frac{dq}{dt} &= \frac{\partial \bar{q}(R)}{\partial R} \dot{R} + \frac{d\delta q}{dt}. \end{aligned} \quad (7)$$

Equation (5) consequently becomes

$$\begin{pmatrix} \frac{d\delta p}{dt} \\ \frac{d\delta q}{dt} \end{pmatrix} = \Gamma_0(R) \left[\begin{pmatrix} \delta p \\ \delta q \end{pmatrix} - \Gamma_0^{-1}(R) \begin{pmatrix} \frac{\partial \bar{p}}{\partial R} \\ \frac{\partial \bar{q}}{\partial R} \end{pmatrix} \dot{R} \right]. \quad (8)$$

Two remarks are necessary for this equation of $(\delta p, \delta q)$. First, because it is already assumed that throughout the protocol $R = R(t)$ the studied energy eigenstates never become degenerate, the corresponding fixed points in the phase space do not vanish or collide. It is therefore legitimate to always associate the deviations with one fixed point so long as $(\delta p, \delta q)$ is small. Second, it can be shown that the determinant $|\Gamma_0|$ does not vanish with non-degenerate energy eigenstates. Γ_0^{-1} in Eq. (8) hence exists for all R .

Remarkably, Eq. (8) possesses a canonical structure. The variables $(\delta p, \delta q)$ are a canonical pair and Eq. (8) can be derived from the following Hamiltonian

$$\begin{aligned} H_1(R, \dot{R}) &= \frac{1}{2} \left(\frac{\partial^2 H_0}{\partial q^2} \right)_{\bar{p}, \bar{q}} (\delta q - B_1)^2 \\ &+ \left(\frac{\partial^2 H_0}{\partial q \partial p} \right)_{\bar{p}, \bar{q}} (\delta q - B_1)(\delta p - A_1) \\ &+ \frac{1}{2} \left(\frac{\partial^2 H_0}{\partial p^2} \right)_{\bar{p}, \bar{q}} (\delta p - A_1)^2, \end{aligned} \quad (9)$$

where $A_1 = A_1(R, \dot{R})$ and $B_1 = B_1(R, \dot{R})$ are defined as

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \Gamma_0^{-1}(R) \begin{pmatrix} \frac{\partial \bar{p}}{\partial R} \\ \frac{\partial \bar{q}}{\partial R} \end{pmatrix} \dot{R}. \quad (10)$$

This expression was previously obtained by Fu and Liu [19]. It is clear that the first-order Hamiltonian (9) describes harmonic oscillations around the central point (A_1, B_1) .

The first-order Hamiltonian H_1 generating the dynamics of $(\delta p, \delta q)$ depends upon two parameters $R(t)$ and $\dot{R}(t)$. We assume that $\dot{R}(t)$ also changes slowly with time. In this case, the dynamics of $(\delta p, \delta q)$ becomes the adiabatic evolution of H_1 and can be understood with the help of the classical adiabatic theorem. We define the action for $(\delta p, \delta q)$ as

$$I_1 = \frac{1}{2\pi} \oint \delta p \cdot d(\delta q). \quad (11)$$

This action is the adiabatic invariant possessed by H_1 [20]. (A_1, B_1) is the fixed point of H_1 with $I_1 = 0$.

The dynamics of $(\delta p, \delta q)$ can be viewed as a spiral motion along the adiabatic trajectory specified by fixed point (A_1, B_1) . The amplitude of the spiral oscillations is controlled by the action I_1 . With this analysis, it becomes clear that when both $R(t)$ and $\dot{R}(t)$ change slowly with time (A_1, B_1) describes an adiabatic trajectory shifted from the ideal trajectory of fixed point $[\bar{p}(R), \bar{q}(R)]$ as shown in Fig. 1.

We now consider two typical cases. In the first case, \dot{R} is increased slowly from zero. In this case, as A_1 and B_1 are zero initially, the action I_1 is zero and the adiabatic evolution to the first order will follow exactly the adiabatic trajectory specified by (A_1, B_1) . This is illustrated in Fig. 2(1). In the second case, the external driving rate \dot{R} is finite and small at the beginning. This means that (A_1, B_1) is not zero initially and the action I_1 has a finite and small value. In this second case, the adiabatic evolution will become a spiral motion around the trajectory of (A_1, B_1) as shown in Fig. 2(2). This analysis of the second case in fact implies that infrequent sudden but small jump of \dot{R} will not break down the adiabaticity of the evolution. Note that the smallness of the jump in $\dot{R}(t)$ is implicitly guaranteed by the slow change of $R(t)$. We mention it explicitly in our discussion just for clarity.

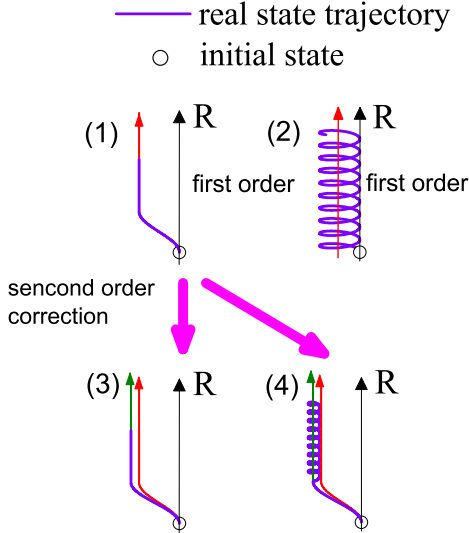


FIG. 2: (Color online) Adiabatic evolutions at first and second orders. The black line is the zeroth-order adiabatic trajectory, the red line the first-order adiabatic trajectory, and the dark green line the second-order adiabatic trajectory. (1) The evolution follows the first-order adiabatic trajectory when the adiabatic manipulation is gradually launched (continuous increasing of \dot{R} from zero); (2) it becomes a spiral oscillatory motion when the process is started with a finite \dot{R} . (3) The state follows the second-order adiabatic trajectory when \ddot{R} is changed slowly from zero; (4) it becomes a spiral-like motion when \ddot{R} is started with a finite value.

Our first-order adiabatic theory shows that a small

quantum transition to other energy eigenstates always occurs with probability proportional to \dot{R} . The probability is zero only in special cases where the coefficients in Eq. (10) vanish.

Our first-order theory offers a deep insight into the generic subtlety of how the adiabatic following breaks down. Let us consider a situation where $\dot{R}(t)$ is small but changes with a great rate, i.e., $\ddot{R}(t)$ is large. In this case, the dynamics governed by H_1 is not adiabatic; I_1 is not an adiabatic invariant and can not stay small for a long time. When the evolution is long enough, the dynamical evolution of the first-order deviations $(\delta p, \delta q)$ will no longer be bounded: the small deviations $(\delta p, \delta q)$ can accumulate and eventually be amplified to the zeroth-order level. This breakdown due to the largeness of $\ddot{R}(t)$ clearly depends on the detail of the protocol $R(t)$ and the Hamiltonian; general conclusions will be difficult to reach.

We note that our theory can be naturally extended to a Hilbert space of larger dimension $n > 2$, where the matrix Γ_0 becomes $2(n-1) \times 2(n-1)$ dimension and the first-order Hamiltonian has $(n-1)$ pairs of canonical variables.

IV. SECOND ORDER DEVIATIONS

In the previous section we have found that the first-order correction $(\delta p, \delta q)$ evolves according to a first-order Hamiltonian H_1 . It is natural to wonder whether we can find a similar Hamiltonian for the second-order deviations. We find that if the system follows the first-order adiabatic trajectory (see Fig. 2(1)), we can indeed find such a Hamiltonian. We write

$$p = \bar{p} + A_1 + \delta^2 p, \quad q = \bar{q} + B_1 + \delta^2 q. \quad (12)$$

After substituting it into H_0 and with straightforward calculation, we obtain the second-order Hamiltonian

$$\begin{aligned} H_2(R, \dot{R}, \ddot{R}) = & \frac{1}{2} \left(\frac{\partial^2 H_0}{\partial q \partial q} \right)_{\bar{p}+A_1, \bar{q}+B_1} (\delta^2 q - B_2)^2 \\ & + \left(\frac{\partial^2 H_0}{\partial q \partial p} \right)_{\bar{p}+A_1, \bar{q}+B_1} (\delta^2 q - B_2)(\delta^2 p - A_2) \\ & + \frac{1}{2} \left(\frac{\partial^2 H_0}{\partial p \partial p} \right)_{\bar{p}+A_1, \bar{q}+B_1} (\delta^2 p - A_2)^2, \end{aligned} \quad (13)$$

where

$$\begin{aligned} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = & \Gamma_0^{-1} \left[\begin{pmatrix} \frac{\partial A_1}{\partial R} \\ \frac{\partial B_1}{\partial R} \end{pmatrix} \dot{R} + \begin{pmatrix} \frac{\partial A_1}{\partial \dot{R}} \\ \frac{\partial B_1}{\partial \dot{R}} \end{pmatrix} \ddot{R} \right] \\ & - \frac{1}{2} \Gamma_0^{-1} \delta \Gamma \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}. \end{aligned} \quad (14)$$

Here $\delta \Gamma$ is defined as

$$\delta \Gamma = \left(\frac{\partial \Gamma}{\partial p} \right)_{\bar{p}, \bar{q}} A_1 + \left(\frac{\partial \Gamma}{\partial q} \right)_{\bar{p}, \bar{q}} B_1 \quad (15)$$

with

$$\Gamma \equiv \begin{pmatrix} -\frac{\partial^2 H_0}{\partial q \partial p} & -\frac{\partial^2 H_0}{\partial q \partial q} \\ \frac{\partial^2 H_0}{\partial p \partial p} & \frac{\partial^2 H_0}{\partial p \partial q} \end{pmatrix}. \quad (16)$$

The detailed derivation of this second-order Hamiltonian (13) can be found in Appendix A along with some subtlety involved in the derivation.

The second-order Hamiltonian H_2 has a similar structure as H_1 and describes a generalized harmonic oscillator. The significant difference is that H_2 depends on three parameters (R, \dot{R}, \ddot{R}) while H_1 depends on only two parameters (R, \dot{R}). In the following, we conduct a similar analysis for H_2 as for H_1 . We focus on the case where \ddot{R} , along with R, \dot{R} , changes slowly with time. In this case, the dynamics of the second-order deviation ($\delta^2 p, \delta^2 q$) as governed by H_2 is adiabatic. We define the action for ($\delta^2 p, \delta^2 q$) as

$$I_2 = \frac{1}{2\pi} \oint \delta^2 p \cdot d(\delta^2 q), \quad (17)$$

which is the adiabatic invariant possessed by H_2 [20]. (A_2, B_2) is the fixed point of H_2 with $I_2 = 0$. The dynamics of ($\delta^2 p, \delta^2 q$) can be viewed as a spiral motion along the adiabatic trajectory specified by fixed point (A_2, B_2) . The amplitude of the spiral oscillations is controlled by the action I_2 . It is clear from this analysis that (A_2, B_2) describes an adiabatic trajectory shifted from the first-order one that is specified by $[\bar{p} + A_1, \bar{q} + B_1]$ (see Fig. 1).

We again consider two typical cases. (i) When both \dot{R} and \ddot{R} are started continuous from zero, I_2 is zero and the dynamics of ($\delta^2 p, \delta^2 q$) follows exactly (A_2, B_2) . This means that the state follows exactly the adiabatic trajectory deviating from original instantaneous eigenstate by $(A_1 + A_2, B_1 + B_2)$ (see Fig. 2(3)). (ii) When the system starts with a finite \ddot{R} , I_2 is nonzero and the system undergoes a spiral motion around (A_2, B_2) (see Fig. 2(4)). The amplitude of the spiral motion is controlled by I_2 .

We can continue this procedure and construct a k th-order Hamiltonian for the k th-order deviation. The result and the detailed derivation can be found in Appendix B. A general feature is that the k th-order Hamiltonian will depend on $k + 1$ parameters, $R, \dot{R}, \ddot{R}, \dots, d^k R/dt^k$, and the adiabaticity of its dynamics is controlled by these parameters. We note that a k th-order Hamiltonian can be constructed only when the dynamics of the deviations of order $(k - 1)$ follows the $(k - 1)$ th-order adiabatic trajectory (the scenarios illustrated in Fig. 2(1,3)).

In summary, we have developed a hierarchical theory for quantum adiabatic evolution. In this theory, a hierarchy of Hamiltonians can be constructed: the k th-order deviation from quantum adiabatic theorem is governed by a k th-order Hamiltonian. This theory not only offers explicit formula to compute the deviations of various orders but also presents an intuitive insight into the intricacy of adiabatic evolution. To illustrate the latter, we use the second-order Hamiltonian $H_2(R, \dot{R}, \ddot{R})$ as

an example. We assume that R, \dot{R} is small while \ddot{R} is large. In this case the dynamics of the second-order deviation ($\delta^2 p, \delta^2 q$) governed by H_2 is not adiabatic. As a result, the second-order deviation ($\delta^2 p, \delta^2 q$) can grow, reach the first-order level, and continue to grow even bigger. The evolution of the first-order deviations is adiabatic due to the smallness of R and \dot{R} . However, this conclusion is only true when the deviation is small. If the second-order deviation grows so large that the deviation is no longer small, the adiabaticity at the first-order level is then broken down. Eventually, the growth starting from the second-order level can even break down the zeroth-order adiabaticity. This example shows that the adiabatic evolution can be maintained for an infinite long time only when all orders of derivative of R with respect to time are small. However, this kind of growth of deviation due to high-order non-adiabaticity takes a very long time, which is usually beyond the physically relevant time scale. So, we do not need to worry about it most of time when applying in real physical problems. As the exact time scale for this growth depends on the detail of the control protocol $R(t)$, it can only be computed case by case.

V. TWO EXAMPLES

We now use two simple systems to illustrate our hierarchical theory. One is a spin-1/2 particle in an external rotating magnetic field; the other is the Landau-Zener model. They are chosen because they are either exactly solvable or their numerical solutions can be found with great accuracy. In this way, there will be no ambiguity in checking the validity of our hierarchical theory. In this section, we always assume $\hbar = 1$.

A. spin-1/2 under a rotating field

In the hierarchical theory, the first-order deviation and its dynamics is of the most importance. In this subsection, we employ the simple model of a spin-1/2 particle in a rotating magnetic field to illustrate the first-order adiabatic theory. The Hamiltonian for a spin-1/2 particle in an external rotating field is

$$\hat{H}_0 = \frac{1}{2} \begin{pmatrix} 0 & L \exp(-i\alpha) \\ L \exp(i\alpha) & 0 \end{pmatrix}, \quad (18)$$

where $\alpha(t)$ changes slowly with time for a rotating field. We use $|\psi\rangle = (c_1, c_2)^T$, where c_1 and c_2 are complex, to denote the quantum state of this spin-1/2 particle. We turn to the classical formulation by introducing a pair of conjugate variables, $p = \arg(c_2) - \arg(c_1)$ and $q = |c_2|^2$. The corresponding classical Hamiltonian is

$$H_0 = \langle \psi | \hat{H}_0 | \psi \rangle = L \sqrt{q - q^2} \cos(\alpha - p). \quad (19)$$

The classical Hamiltonian in Eq. (19) has two elliptic fixed points, namely, $(\bar{q} = 1/2, \bar{p} = \alpha)$ and $(\bar{q} = 1/2, \bar{p} =$

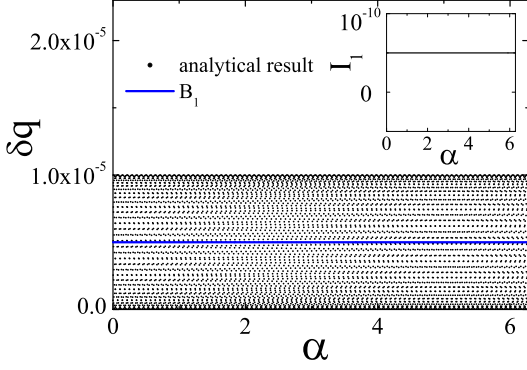


FIG. 3: The first-order solution of a spin-1/2 particle in a slowly rotating magnetic field. The dots are δq computed from the analytical solution to the first order Eq. (22). The solid line is B_1 of the first-order fixed point. The inset shows the first-order action I_1 computed from the analytical solution Eq. (22). $\omega = 10^{-5}$.

$\alpha + \pi$), corresponding respectively to the two eigenstates of Eq. (18). We focus on the adiabatic following of the fixed point $\bar{q} = 1/2, \bar{p} = \alpha$ as α (rotating field) changes slowly. The conventional adiabatic theorem states that the actual state will accurately follow the instantaneous state ($\bar{q} = 1/2, \bar{p} = \alpha$).

On top of the conventional adiabatic theorem, there are first-order corrections. To that end we now derive the effective first-order Hamiltonian H_1 . According to Eqs. (9), (10) and (19), one finds for fixed point ($q = 1/2, p = \alpha$),

$$H_1 = -\frac{L}{2} \left[2(\delta q - \frac{\dot{\alpha}}{2L})^2 + \frac{1}{2}(\delta p)^2 \right]. \quad (20)$$

Interestingly, for this example, H_1 happens to be independent of the adiabatic parameter α . The first-order fixed point is located at $A_1 = 0, B_1 = \dot{\alpha}/2L$. In the following we consider three different control protocols $\alpha(t)$ with $\alpha(0) = 0$ and the initial state emanating exactly from the fixed point $q(0) = 1/2, p(0) = \alpha$.

(i) Let us first consider the simplest protocol in which $\alpha = \omega t$ with ω being constant. At $t = 0$, the initial state is $q = 1/2, p = 0$ while the first-order fixed point is at ($A_1 = 0, B_1 = \omega/2L$). So, the state starts off the first-order fixed point and the first-order action is

$$I_1 = \frac{\omega^2}{4L^2}. \quad (21)$$

According to our theory, the first-order deviation will undergo a spiral motion, similar to what is depicted in Fig. 2(2), with its amplitude controlled by I_1 .

The validity of our theory can be checked by directly integrating the Schrödinger equation governed by (18). This solution can be found exactly. With the omission of

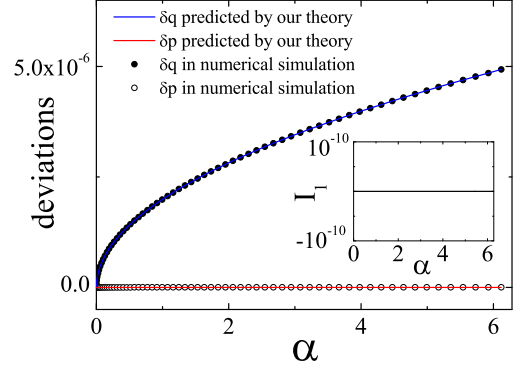


FIG. 4: Numerical results for the first-order correction ($\delta p, \delta q$) obtained from the Hamilton's equation of motion governed by (19). The control protocol is $\alpha = \frac{1}{2}at^2$ with $a = 7.96 \times 10^{-12}$. The dots and circles are numerical results while the solid lines are for the first-order fixed point ($A_1 = 0, B_1 = at/2L$). The inset shows the numerically computed I_1 .

higher orders, the solution can be written as

$$|\psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 - \frac{\omega}{2L} [1 - \cos(Lt)] \\ [1 + \frac{\omega}{2L} (1 - \cos(Lt))] e^{i[\omega t + \frac{\omega}{L} \sin(Lt)]} \end{pmatrix}. \quad (22)$$

This solution is plotted in Fig. 3 by mapping $|\psi\rangle$ to (p, q) and thus to $(\delta p, \delta q)$. In this figure, we clearly see oscillations around the fixed point ($A_1 = 0, B_1 = \omega/2L$), consistent with our first-order theory. As shown in the inset of this figure, our direct computation also confirms that the first-order action I_1 is a constant. We point out that this is equivalent to a system under the following control protocol

$$\alpha = 0 \quad \text{for } t < 0; \quad \alpha = \omega t \quad \text{for } t > 0. \quad (23)$$

That is, there can be a small sudden jump in $\dot{\alpha}$ at $t = 0$. Analytically, the first-order deviation can be readily computed from the solution (22)

$$\begin{aligned} \delta p &= p - \bar{p} = \frac{\omega}{L} \sin(Lt), \\ \delta q &= q - \bar{q} = \frac{\omega}{2L} (1 - \cos(Lt)), \end{aligned} \quad (24)$$

which is indeed consistent with the first-order Hamiltonian dynamics predicted by H_1 in Eq. (20).

(ii) In the second protocol, the speed $\dot{\alpha}$ increases gradually from zero. To be specific, we choose $\alpha = \frac{1}{2}at^2$ with $a = 7.96 \times 10^{-12}$. For this protocol, the first-order fixed point is ($A_1 = 0, B_1 = 0$) at $t = 0$. Therefore, according to our first-order theory, the action $I_1 = 0$ and the dynamics of the first-order deviation ($\delta p, \delta q$) follows exactly the first-order fixed point ($A_1 = 0, B_1 = at/2L$). We have numerically solved the Hamilton's equations of motion governed by Eq. (19) for this second protocol. The numerical results for $(\delta p, \delta q)$ and I_1 are shown in Fig. 4 and an excellent agreement with our first-order theory is found.

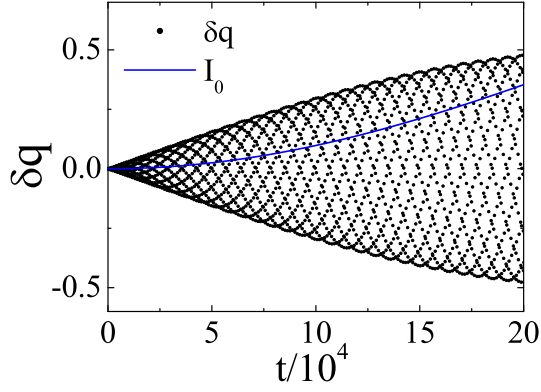


FIG. 5: Numerical solution of δq and $I_0 = \frac{1}{2\pi} \oint p \cdot dq$ with Hamilton's equation of motion governed by (19). For the control protocol, we have $|\dot{\alpha}| = 10^{-5}$. The sign of $\dot{\alpha}$ oscillates with the frequency $\nu = 1$.

(iii) In the third protocol, we change the sign of $\dot{\alpha}$ frequently while keeping $|\dot{\alpha}|$ small. This is to ensure that the second-order time derivative $\ddot{\alpha}$ can be quite large. We use this protocol to illustrate an insight offered by our hierarchical theory: high-order time derivative of R can also lead to the breakdown of adiabaticity. For this spin-1/2 system, the smallness of $|\dot{\alpha}|$ does not guarantee the accuracy of the quantum adiabatic theorem. When $\ddot{\alpha}$ is large, then the first-order dynamics governed by H_1 is no longer adiabatic, and the accumulation of $(\delta p, \delta q)$ will eventually lead to the breakdown of adiabaticity at the zeroth orders. We have solved numerically the equations of motion governed by Eq. (19). The results are plotted in Fig. 5, where we see that δq can indeed grow and destroy the adiabaticity. The solid line seen in the middle of the pattern shown in Fig. 5 demonstrates that the action I_0 is no longer a constant.

B. Hierarchy of adiabatic corrections in the Landau-Zener model

In this subsection, we consider a different model, the Landau-Zener (LZ) model, and use it to demonstrate higher-order deviations. The LZ Hamiltonian can be written as

$$\hat{H}_0^{\text{LZ}} = \frac{1}{2} \begin{pmatrix} z & x \\ x & -z \end{pmatrix}, \quad (25)$$

where the coupling term $x > 0$ is a constant whereas z changes slowly and linearly from $-Z_0$ to Z_0 ,

$$z = Vt, \quad t : -Z_0/V \rightarrow Z_0/V. \quad (26)$$

Similarly, we define $c_1 = |c_1|e^{i\phi_{c_1}}$, $c_2 = |c_2|e^{i\phi_{c_2}}$, $p = \phi_{c_2} - \phi_{c_1}$, and $q = |c_2|^2$, and obtain the classical Hamiltonian (drop a constant):

$$H_0 = \langle \psi | \hat{H}_0^{\text{LZ}} | \psi \rangle = x\sqrt{q - q^2} \cos(p) - zq. \quad (27)$$

This classical Hamiltonian has two fixed points at $(\bar{p} = 0, \bar{q} = \frac{1}{2} - \frac{z}{2\sqrt{x^2+z^2}})$ and $(\bar{p} = \pi, \bar{q} = \frac{1}{2} + \frac{z}{2\sqrt{x^2+z^2}})$. Without loss of generality, we focus on the fixed point $(\bar{p} = \pi, \bar{q} = \frac{1}{2} + \frac{z}{2\sqrt{x^2+z^2}})$, which corresponds to the eigenstate with the lower energy. According to the quantum adiabatic theorem, i.e., zeroth-order theory, when the initial state is the ground state $\left[\cos\left(\frac{\arctan(x/Z_0)}{2}\right), -\sin\left(\frac{\arctan(x/Z_0)}{2}\right) \right]^T$ at $z = -Z_0$ the system will follow the instantaneous eigenstate and ultimately reach $\left[-\sin\left(\frac{\arctan(x/Z_0)}{2}\right), \cos\left(\frac{\arctan(x/Z_0)}{2}\right) \right]^T$ at $z = Z_0$. In what follows, we will compute explicitly the first-order deviation and the second-order deviation, and discuss some general properties of the higher-order deviations.

According to Eqs. (9,27), the first-order Hamiltonian H_1 reads

$$H_1 = \sqrt{x^2 + z^2} \left(1 + \frac{z^2}{x^2} \right) (\delta q)^2 + \frac{1}{4} x^2 \frac{(\delta p - \frac{V}{x^2+z^2})^2}{\sqrt{x^2 + z^2}}. \quad (28)$$

The fixed point for the first-order deviation $(\delta p, \delta q)$ (or the first-order deviation from the zeroth-order adiabatic trajectory) is

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} \frac{V}{x^2+z^2} \\ 0 \end{pmatrix}. \quad (29)$$

The results for the second-order deviation $(\delta^2 p, \delta^2 q)$ can be computed similarly. The second-order Hamiltonian is

$$\begin{aligned} H_2 = & \sqrt{x^2 + z^2} \left(1 + \frac{z^2}{x^2} \right) \left(\delta^2 q - \frac{5x^2 z V^2}{4(x^2 + z^2)^{7/2}} \right)^2 \\ & - \frac{zV}{x^2 + z^2} \left(\delta^2 q - \frac{5x^2 z V^2}{4(x^2 + z^2)^{7/2}} \right) \delta^2 p \\ & + \frac{1}{4} x^2 \frac{(\delta^2 p)^2}{\sqrt{x^2 + z^2}}. \end{aligned} \quad (30)$$

The fixed point (or, the deviation from the first-order adiabatic trajectory) is

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{5x^2 z V^2}{4(x^2 + z^2)^{7/2}} \end{pmatrix};$$

We consider the limit $Z_0 \rightarrow \infty$. At this limit, we have $A_1 = B_1 = A_2 = B_2 = 0$ at $|z| = \infty$. This means that the deviations of the first-order and the second-order are zero both at the beginning and at the end of the evolution. The higher-order deviations can also be computed with the formula in Appendix B. There is no need to write them down here. We only want to mention, for all these higher-order deviations, we also have

$$A_k \rightarrow 0; \quad B_k \rightarrow 0, \quad \text{as } |z| \rightarrow \infty. \quad (31)$$

This indicates that the LZ tunneling rate at $Z_0 \rightarrow \infty$ tends to zero to all orders of the small driving rate V based on our hierarchy theory. This is perfectly consistent with the standard rigorous result for the LZ tunneling rate $\exp(-\frac{\pi x^2}{V})$ [23], where any term in the Taylor expansion of $\exp(-\frac{\pi x^2}{V})$ with respect to V is zero. This result is in sharp contrast to the previous case in the last subsection, where the leading term of the deviation from an ideal adiabatic behavior is proportional to ω^2 .

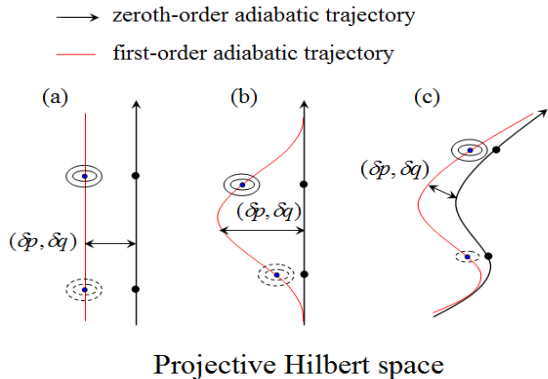


FIG. 6: (color online) Schematics of different scenarios for the first-order deviation from the zeroth-order adiabatic trajectory. (a) For the case of a spin-1/2 particle under a rotating field considered in Sec. V.A, the first-order deviation from the zeroth-order adiabatic trajectory is a constant. (b) In the case of a LZ process considered in Sec. V.B, the average deviation in either the initial stage or the final stage approaches zero, but it can be appreciable at the intermediate stage. (c) The first-order deviations $(\delta p, \delta q)$ can be manipulated by designing the time dependence of $R(t)$ and $\dot{R}(t)$.

We now summarize this section with Fig. 6, where the

first-order deviations discussed above are schematically plotted. It is clear from our theory that the first-order deviations can be manipulated by designing $R(t)$ and $\dot{R}(t)$. This can be very useful to control the nonadiabatic error in quantum adiabatic computation [24]. We plan to pursue this issue in the near future.

VI. CONCLUSION

In this work, we have studied the quantum adiabatic evolution and developed a hierarchical quantum theory for the small deviations from the conventional quantum adiabatic theorem. The claim from the theorem that no population transitions between non-degenerate instantaneous energy eigenstates is true only when the external driving is infinitely slow. For a small and nonzero driving rate of the adiabatic parameter, there are small deviations, i.e., small transitions between different energy eigenstates. We have found that the deviations of k th-order are governed by a k th-order Hamiltonian. Our approach can be directly applied to classical adiabatic processes and nonlinear quantum adiabatic evolution on the mean-field level [25, 26]. It is of considerable interest to apply our findings to assist in the control of adiabatic processes in both classical and quantum systems [27–29].

Acknowledgments

This work is supported by the NBRP of China (2013CB921903, 2012CB921300) and the NSF of China (11105123, 11274024, 11334001).

-
- [1] M. Born and V. A. Fock, *Zeitschrift für Physik A* **51**, 165 (1928).
 - [2] M. Maamache and Y. Saadi, *Phys. Rev. A* **78**, 052109 (2008); M. Maamache and Y. Saadi, *Phys. Rev. Lett.* **101**, 150407 (2008).
 - [3] G. Rigolin and G. Ortiz, *Phys. Rev. A* **85**, 062111 (2012); G. Rigolin and G. Ortiz, *Phys. Rev. Lett.* **104**, 170406 (2010).
 - [4] D.M. Tong, K. Singh, L.C. Kwek, and C.H. Oh, *Phys. Rev. Lett.* **95**, 110407 (2005).
 - [5] T. T. Nguyen-Dang, E. Sinelnikov, A. Keller, and O. Atabek, *Phys. Rev. A* **76**, 052118 (2007).
 - [6] C.P. Sun, *Phys. Rev. D* **41**, 1318 (1990); Z. Wu, *Phys. Rev. A* **40**, 6852 (1989).
 - [7] V. I. Yukalov, *Phys. Rev. A* **79**, 052117 (2009).
 - [8] K. P. Marzlin and B. C. Sanders, *Phys. Rev. Lett.* **93**, 160408 (2004).
 - [9] J. Ortigoso, *Phys. Rev. A* **86**, 032121 (2012); M. H. S. Amin, *Phys. Rev. Lett.* **102**, 220401 (2009); R. MacKenzie, A. Morin-Duchesne, H. Paquette, and J. Pinel, *Phys. Rev. A* **76**, 044102 (2007).
 - [10] D. Comparat, *Phys. Rev. A* **80**, 012106 (2009).
 - [11] Y. Zhao, *Phys. Rev. A* **77**, 032109 (2008); J. Ma, Y. Zhang, E. Wang, and B. Wu, *Phys. Rev. Lett.* **97**, 128902 (2006); S. Duki, H. Mathur, and O. Narayan, *Phys. Rev. Lett.* **97**, 128901 (2006); Z. Wu and H. Yang, *Phys. Rev. A* **72**, 012114 (2005); J. Du, L. Hu, Y. Wang, J. Wu, M. Zhao, and D. Suter, *Phys. Rev. Lett.* **101**, 060403 (2008); D. M. Tong, *Phys. Rev. Lett.* **104**, 120401 (2010); A. Ambainis and O. Regev, *quant-ph/0411152*.
 - [12] E. Farhi, J. Goldstone, S. Gutmann, J. Lapan, A. Lundgren, and D. Preda, *Science* **292**, 472 (2000).
 - [13] Andrew M. Childs, Edward Farhi, and John Preskill, *Phys. Rev. A* **65**, 012322 (2001).
 - [14] S. Weinberg, *Ann. of Phys. (N.Y.)* **194**, 336 (1989); A. Hestenes, *Phys. Rev. D* **31**, 1341 (1985).
 - [15] J. Liu, B. Wu, and Q. Niu, *Phys. Rev. Lett.* **90**, 170404 (2003).
 - [16] M. V. Berry and M. A. Morgan, *Nonlinearity* **9**, 787 (1996).

- [17] A. D. A. M. Spallicci, A. Morbidelli, and G. Metris, Non-linearity **18**, 45 (2005).
- [18] M. V. Berry and J. M. Robbins, Proc. Roy. Soc. Lond. **A442**, 641 (1993).
- [19] J. Liu and L.B. Fu, Phys. Rev. A **81**, 052112 (2010); L.B. Fu and J. Liu, Ann. Phys. **325**, 2425 (2010).
- [20] P.A.M. Dirac, Proc. R. Soc. **107**, 725 (1925).
- [21] Bohm Mostafazadeh *et al.*, The geometric phase in quantum systems, Springer, 225-243 (2003).
- [22] Q. Zhang, J. B. Gong, and C. H. Oh, Ann. Phys. **327**, 1202 (2012); Q. Zhang, J. Phys. A **45**, 295302 (2012).
- [23] L.D. Landau, Phys. Z. Sowjetunion **2**, 46 (1932); C. Zener, Proc. R. Soc. A **137**, 696 (1932).
- [24] LiXiang Cen, XinQi Li, YiJing Yan, HouZhi Zheng, and ShunJin Wang, Phys. Rev. Lett. **90**, 147902 (2003); Yu Shi and Yong-Shi Wu, Phys. Rev. A **69**, 024301 (2004);
- [25] Q. Zhang, J. B. Gong, and C. H. Oh, Phys. Rev. Lett. **110**, 130402 (2013).
- [26] V.I. Yukalov, Phys. Rev. A **79**, 052117 (2009); S.Y. Meng, L.B. Fu, and J. Liu, *ibid.* **78**, 053410 (2008); A.P. Itin and S. Watanabe, Phys. Rev. Lett. **99**, 223903 (2007).
- [27] C. Jarzynski, Phys. Rev. A **88**, 040101(R) (2013).
- [28] J. W. Deng, Q.-h. Wang, Z. H. Liu, P. Hanggi, and J. B. Gong, Phys. Rev. E **88**, 062122 (2013).
- [29] S. Deffner, C. Jarzynski, and A. del Campo, arXiv:1401.1184.

Appendix A: Detailed derivations for the second-order theory

The premise of dealing with the second-order deviation is that the state is around the first-order fixed point. This allows us to express $(\delta p, \delta q)$ as the following,

$$\delta p = \delta^2 p + A_1; \quad \delta q = \delta^2 q + B_1, \quad (\text{A1})$$

where $\delta^2 p$ and $\delta^2 q$ describe the actual dynamics of $(\delta p, \delta q)$ on top of their time-averaged values (A_1, B_1) .

Note that in deriving H_1 we have only kept the first-order term when expanding the force field $\left[-\frac{\partial H_0(R)}{\partial q}, \frac{\partial H_0(R)}{\partial p}\right]$. This is adequate for the first-order theory. When considering the second-order deviation, we should also keep the second-order terms in the expansion. Specifically, substituting Eq. (A1) into Eqs. (5,8), keeping the second-order expansion terms

$$\frac{1}{2} \left(\delta p \frac{\partial}{\partial p} + \delta q \frac{\partial}{\partial q} \right)^2 H'_0 \quad H'_0 = \frac{-\partial H_0}{\partial q} \quad \text{or} \quad \frac{\partial H_0}{\partial p}, \quad (\text{A2})$$

and neglecting terms containing $[\delta^2 p]^2$ or $[\delta^2 q]^2$ (which are fourth-order), one finds (employing Eq. (10))

$$\begin{pmatrix} \frac{d\delta^2 p}{dt} \\ \frac{d\delta^2 q}{dt} \end{pmatrix} = \frac{1}{2} \delta \Gamma \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} + (\Gamma_0 + \delta \Gamma) \begin{pmatrix} \delta^2 p \\ \delta^2 q \end{pmatrix} - \begin{pmatrix} \frac{dA_1}{dt} \\ \frac{dB_1}{dt} \end{pmatrix}, \quad (\text{A3})$$

where $\delta \Gamma$ is defined in Eq. (15) as the state under consideration shifts from (\bar{p}, \bar{q}) to $(\bar{p} + A_1, \bar{q} + B_1)$.

Rearranging some terms on the right-hand side of Eq. (A3), we arrive at

$$\begin{pmatrix} \frac{d\delta^2 p}{dt} \\ \frac{d\delta^2 q}{dt} \end{pmatrix} = (\Gamma_0 + \delta \Gamma) \left\{ \begin{pmatrix} \delta^2 p \\ \delta^2 q \end{pmatrix} - (\Gamma_0 + \delta \Gamma)^{-1} \begin{pmatrix} \frac{dA_1}{dt} \\ \frac{dB_1}{dt} \end{pmatrix} + \frac{1}{2} (\Gamma_0 + \delta \Gamma)^{-1} \delta \Gamma \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \right\}. \quad (\text{A4})$$

The fixed-point solution for $\delta^2 p$ and $\delta^2 q$ can be found from Eq. (A4); it is

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \Gamma_0^{-1}(R) \left[\begin{pmatrix} \frac{\partial A_1}{\partial R} \\ \frac{\partial B_1}{\partial R} \end{pmatrix} \dot{R} + \begin{pmatrix} \frac{\partial A_1}{\partial V} \\ \frac{\partial B_1}{\partial V} \end{pmatrix} \ddot{R} \right] - \frac{1}{2} \Gamma_0^{-1} \delta \Gamma \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}, \quad (\text{A5})$$

where the time derivatives of the adiabatic parameter R , \dot{R} and \ddot{R} , are assumed to be in the same order of magnitude. All higher-order terms, such as those terms of the order of \dot{R}^j with $j \geq 3$, are neglected. Under this treatment, it is now seen that, in terms of their time-averaged values, a more accurate prediction of $(\delta p, \delta q)$ is given by $(A_1 + A_2, B_1 + B_2)$. Note that A_2 and B_2 are evidently proportional to $\propto \dot{R}^2$. Equations (A4, A5) are just the second-order dynamics and the second-order fixed point given in the main text (see Eqs. (13) and (14)). One can now readily write down the second-order Hamiltonian

$$\begin{aligned} H_2(R, \dot{R}) &= \frac{1}{2} \left(\frac{\partial^2 H_0}{\partial q^2} \right)_{p_1, q_1} (\delta^2 q - B_2)^2 \\ &+ \left(\frac{\partial^2 H_0}{\partial q \partial p} \right)_{p_1, q_1} (\delta^2 q - B_2)(\delta^2 p - A_2) \\ &+ \frac{1}{2} \left(\frac{\partial^2 H_0}{\partial p^2} \right)_{p_1, q_1} (\delta^2 p - A_2)^2, \end{aligned} \quad (\text{A6})$$

One only need to note that (p, q) take value of $(\bar{p} + A_1, \bar{q} + B_1)$ instead of (\bar{p}, \bar{q}) as we are at the second-order approximation.

Appendix B: High-order deviations in quantum adiabatic evolution

The dynamics of the k th-order deviation $(\delta^k p, \delta^k q)$ can be derived iteratively by substituting $\delta p = A_1 + A_2 + \dots + \delta^k p$ and $\delta q = B_1 + B_2 + \dots + \delta^k q$ into Eqs. (5,8) with the expansion up to the k th-order, provided the fixed points of all the previous $(k-1)$ orders have been obtained. Specifically, $(\delta^3 p, \delta^3 q)$ can be described by a third-order Hamiltonian $H_3(R, \dot{R}, \ddot{R}, \frac{d^3 R}{dt^3})$. The k th-order deviation $(\delta^k p, \delta^k q)$ forms a pair of canonical variables of a k th-order Hamiltonian $H_k(R, \dot{R}, \ddot{R}, \dots, \frac{d^k R}{dt^k})$, demonstrating

that the k th-order deviation will undergo adiabatic evolution only if the time derivatives of parameter R up to the k th-order are all manipulated very slowly in comparison with the intrinsic frequency ω_k of the k th-order Hamiltonian, which is proportional to $|\Gamma_k| \approx |\Gamma_0|$.

The k th order deviation consists of k terms, with the first one associated with the ideal matrix Γ_0 and the adiabatic evolution of the $(k-1)$ th-order deviation $(\delta^{k-1}p, \delta^{k-1}q)$, the second one associated with $\delta\Gamma$ and the evolution of $(\delta^{k-2}p, \delta^{k-2}q)$, and the k th one associated with $\delta^{k-1}\Gamma$ and the zeroth order adiabatic evolution of (\bar{p}, \bar{q}) . The sum of the k terms is the result for the dynamical fixed point of H_k .

To illustrate that a general k th order theory is possible, we consider here only a rather simple case where \dot{R} is a constant. However, even in this case our expressions appear to be complicated and hence readers may skip the technical details (we present them just for completeness). In particular, the k th-order fixed point is

$$\begin{pmatrix} A_k \\ B_k \end{pmatrix} = \Gamma_0^{-1} \begin{pmatrix} \frac{\partial A_{k-1}}{\partial R} \\ \frac{\partial B_{k-1}}{\partial R} \end{pmatrix} \dot{R} - \Gamma_0^{-1} \sum_{j=1}^{k-1} \Delta^j \Gamma \begin{pmatrix} A_{k-j} \\ B_{k-j} \end{pmatrix}. \quad (\text{B1})$$

The deviations $\Delta^j \Gamma$ in Eq. (B1) is defined as

$$\Delta^j \Gamma = \mathcal{T}^j \left\{ \sum_{i=1}^j \frac{1}{(i+1)!} \left[\sum_{r=1}^j (A_r) \frac{\partial}{\partial p} + \sum_{r=1}^j (B_r) \frac{\partial}{\partial q} \right]^i \Gamma \right\} \quad (\text{B2})$$

The function $\mathcal{T}^j(\dots)$ in (B2) is to take the j th-order

terms in (\dots) , i.e., taking the sum of all the terms of the kind $A_t^u B_s^v$ with $tu + sv = j$. For example, A_2 and B_2 are second-order terms in terms of \dot{R} , and A_2^2 and $A_2 B_2$ become the fourth-order terms, so $\mathcal{T}^2(A_2 + B_2 + A_2^2 + A_2 B_2) = A_2 + B_2$, $\mathcal{T}^3(A_2 + B_2 + A_2^2 + A_2 B_2) = 0$ and $\mathcal{T}^4(A_2 + B_2 + A_2^2 + A_2 B_2) = A_2^2 + A_2 B_2$, etc. Specifically, when $j = 1$, $\Delta\Gamma = \frac{1}{2}\delta\Gamma$.

In the case of nonconstant adiabatic speed V , we should include the derivatives of the kind $(d^0 R/dt^0 \equiv R)$

$$\sum_{j=0}^{k-1} \left(\frac{\frac{\partial A_{k-1}}{\partial (d^j R/dt^j)}}{\frac{\partial B_{k-1}}{\partial (d^j R/dt^j)}} \right) \cdot \frac{d^{j+1} R}{dt^{j+1}}$$

for the k th-order deviation.

Generally, the hierarchy adiabatic theory can also be naturally extended to n -mode quantum system by expanding the Γ matrix from dimension 2×2 to dimension $2(n-1) \times 2(n-1)$.

Finally, it is necessary to make three remarks on high-order deviations. First, the deviations of all orders are obtained with respect to what the usual quantum adiabatic theorem predicts. This is the reason that Eq. (B2) looks complicated. Second, we assume that all orders of time derivatives of R , \dot{R} , \ddot{R} , \dots , $d^k R/dt^k$, are of the same order of magnitude. The k th-order term is proportional to \dot{R}^k . Third, in deriving the k th-order deviation in (B1), we have already assumed the adiabaticity holds for up to the k th-order Hamiltonian.